

Active Brownian Motion Models and Applications to Ratchets

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Abstract. We give an overview over recent studies on the model of Active Brownian Motion (ABM) coupled to reservoirs providing free energy which may be converted into kinetic energy of motion. First, we present an introduction to a general concept of active Brownian particles which are capable to take up energy from the source and transform part of it in order to perform various activities. In the second part of our presentation we consider applications of ABM to ratchet systems with different forms of differentiable potentials. Both analytical and numerical evaluations are discussed for three cases of sinusoidal, staircase-like and Mateos ratchet potentials, also with the additional loads modeled by tilted potential structure. In addition, stochastic character of the kinetics is investigated by considering perturbation by Gaussian white noise which is shown to be responsible for driving the directionality of the asymptotic flux in the ratchet. This *stochastically driven directionality* effect is visualized as a strong nonmonotonic dependence of the statistics of the right versus left trajectories of motion leading to a net current of particles. Possible applications of the ratchet systems to molecular motors are also briefly discussed.

PACS. 05.40.-a Fluctuation phenomena, random processes, noise, Brownian motion – 05.45.-a Nonlinear dynamics and chaos

1 Introduction

The study of mechanical systems with support of energy goes back to the investigations of Helmholtz and Rayleigh on the origin of sustained oscillations. Generalizations of the "active friction" introduced by Rayleigh found many applications including the concept of the Active Brownian Motion (ABM) which extends the notion of standard Brownian motion as studied by Einstein, Smoluchowski, Fokker, Planck and others [1] to the field of driven motions [2,3,4,5,6] including a developing theory of swarming motions [7,8,9,11,12].

In this work we first introduce a model of Langevin dynamics coupled to energy depot dynamics and study basic properties. The inclusion of the depot dynamics should model the general observation that external energy which is needed for acceleration of motion is in most cases stored first in a depot or reservoir (a kind of an energy tank) and, only in a second step, becomes converted by a kind of motor into motion. This storage and subsequent conversion of the energy into mechanical work is modeled here in the simplest possible way by a balance equation. Next we study more specific applications to transport problems on Hamiltonian ratchets and discuss applications to molecular motors.

Since the fundamental work of Marian Smoluchowski [1] the problem of transport on ratchets is under a constant debate. Some of the most interesting applications are related to biological problems (see e.g. Jülicher and Prost,[13,14]). Here we will discuss several problems related to the ABM of particles on ratchet potentials. Further we will discuss possible use of ABM in modelling the functioning of ATP and ADP in cells and the related transport mechanisms, having in mind possible applications to biological systems as e.g. proton pumps and electron pumps. Some further relations with the stepping motor described e.g. by Bier [15,17] are also proposed.

2 Model of Brownian motion coupled to energy reservoirs

2.1 Coupling between Langevin dynamics and energy depot dynamics

We postulate dynamics of Brownian particles as determined by the Langevin equation according to a model proposed by Schweitzer et al. [4]:

$$\dot{\mathbf{r}}_i = \mathbf{v}_i; \quad m\dot{\mathbf{v}}_i + \nabla U(\mathbf{r}) = \mathbf{F}_i + \sqrt{2D}\xi(t) \quad (1)$$

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where $U(\mathbf{r})$ is the potential of the conservative forces and $\sqrt{2D}\xi(\mathbf{t})$ is a stochastic force with strength D and a δ -correlated time dependence:

$$\langle \xi_i(t) \rangle = 0; \quad \langle \xi_i(t) \xi_j(t') \rangle = \delta(t - t') \delta_{ij} \quad (2)$$

The driving forces on the RHS of Eq.(1) are expressed in the form [4]

$$\mathbf{F}_i = -m\gamma\mathbf{v} + mde(t)\mathbf{v} \quad (3)$$

where the first term stands for the dissipative force and the second is responsible for the acceleration of movement due to the conversion of the depot energy into kinetic energy of motion. Under the equilibrium conditions, the friction coefficient γ (here defined as the velocity dependent function $\gamma(\mathbf{v})$) is a constant directly related to the noise strength D by the Einstein relation $D = mk_B T \gamma$. Depot energy dissipation and coupling of energy reservoir to the kinetic degrees of freedom give rise to the time-dependent balance equation for $e(t)$

$$\dot{e}(t) = q - ce(t) - de(t)\mathbf{v}^2 \quad (4)$$

Here q is the take-up of energy term and $ce(t)$ describes the internal dissipation in the reservoir which is assumed to be proportional to the depot energy $e(t)$. The conversion of depot into kinetic energy of motion is controlled by the rate d and depends (quadratically) on the actual velocity of the particle. The overall time variation of the mechanical energy of the particle can be derived from Eqs.(1-4) and yields

$$\begin{aligned} \frac{d}{dt} \left(\frac{m}{2} v^2 + U(\mathbf{r}) \right) &= \mathbf{F}_i \mathbf{v}_i + \sqrt{2D} \xi(t) \mathbf{v}_i = \\ &= -\frac{d}{dt} me(t) + m(q - ce(t)) - m\mathbf{v}_i^2 \gamma + \sqrt{2D} \xi(t) \mathbf{v}_i \end{aligned} \quad (5)$$

In an adiabatic approximation (assumed rapid relaxation of variations in $e(t)$ to its stationary value, i.e. $\dot{e}(t) = 0$) we may substitute the energy $e(t)$ in Eq. (3) by its stationary value and get a general form for the dissipative force

$$\mathbf{F}_i = -m\gamma(v_i^2)\mathbf{v}_i \quad (6)$$

The function $\gamma(v^2)$ denotes a velocity-dependent friction, which in our model has a negative part. Accordingly, the depot model [4,6] for the energy supply leads to

$$\gamma(\mathbf{v}^2) = \left(\gamma - \frac{dq}{c + dv^2} \right) \quad (7)$$

where c, d, q are certain positive constants characterizing the energy flows from the depot to the particles. Depending on the parameters γ, c, d and q the dissipative force function may have one zero at $\mathbf{v} = 0$ or two more zeros at

$$\mathbf{v}_0^2 = \beta, \quad (8)$$

when the bifurcation parameter

$$\beta = \frac{q}{\gamma} - \frac{c}{d} \quad (9)$$

becomes positive. In this case a finite characteristic velocity v_0 exists which determines an attractor of motion and one speaks of an active Brownian-particles motion. For $|\mathbf{v}| < v_0$, the dissipative force is positive, i.e. the particle is provided with additional free energy. Hence, slow particles are accelerated, while the motion of fast particles becomes damped. Note that in the case of thermal equilibrium systems we have $\gamma(\mathbf{v}^2) = \gamma_0 = \text{const}$. The adiabatic treatment of the equations proposed by Schweitzer et al. [4] found many applications to problems of active Brownian motions as e.g. swarm dynamics [19,21,22,23]. However, in some cases, and in particular for applications to ratchet problems the adiabatic approximation understood as mere adiabatic elimination of fast variables from the dynamic equations of motion may lead to improper conclusions as will be discussed in the forthcoming paragraphs.

2.2 Free Brownian particles and the action of a constant external force

Let us first discuss the free motion of active particles in a one or two-dimensional space, $\mathbf{r} = \{x_1, x_2\}$. Under the condition of a quasi-stationary depot, $\dot{e}(t) = 0$, the long time (stationary) probability distribution function of the Fokker-Planck equation

$$\begin{aligned} \frac{\partial P(\mathbf{r}, \mathbf{v}, t)}{\partial t} + \mathbf{v} \frac{\partial P(\mathbf{r}, \mathbf{v}, t)}{\partial \mathbf{r}} + \frac{\nabla U(\mathbf{r})}{m} \frac{\partial P(\mathbf{r}, \mathbf{v}, t)}{\partial \mathbf{v}} \\ = \frac{\partial}{\partial \mathbf{v}} \left[\gamma(\mathbf{r}, \mathbf{v}) \mathbf{v} P(\mathbf{r}, \mathbf{v}, t) + D_v \frac{\partial P(\mathbf{r}, \mathbf{v}, t)}{\partial \mathbf{v}} \right] \end{aligned} \quad (10)$$

corresponding to the Langevin equation Eq.(1) with $U(\mathbf{r}) \equiv 0$ can be easily found and reads [6]

$$P_0(\mathbf{v}) = C \left(1 + \frac{dv^2}{c} \right)^{(q/2D_v)} \exp \left[-\frac{\gamma}{2D_v} v^2 \right], \quad (11)$$

where $D_v = D/m^2$ (cf. Eqs. (1,2)) stands for the diffusion coefficient in the velocity space. Accordingly, the mean square displacement

$$\begin{aligned} \langle (\mathbf{r}_1(t) - \mathbf{r}_1(0))^2 \rangle = \\ \int_0^\infty dt_1 \int_0^\infty dt_2 \langle \mathbf{v}(t_1) \mathbf{v}(t_2) \rangle \end{aligned} \quad (12)$$

can be evaluated and in the limit of a strong, supercritical influx of energy ($q \rightarrow \infty$) and for times much longer than $v_0^2/2D_v$ leads to an approximate expression

$$\begin{aligned} \langle (\mathbf{r}_1(t) - \mathbf{r}_1(0))^2 \rangle &= \frac{v_0^4}{D_v} (2t) = 2D_{eff} t = \\ &= \frac{2v_0^4 m^2}{D} t. \end{aligned} \quad (13)$$

So far the usual Brownian motion and the active Brownian motion seem to behave in a quite similar way: we see that the dispersion of the displacement grows linearly

with time resembling typical character of the diffusive motion with $D_{eff} = v_0^4/D_v$. However, the prefactor $2D_{eff}$ is completely different from the value $2k_B T(m\gamma)^{-1}$ which rules the relation $\langle (\mathbf{r}_1(t) - \mathbf{r}_1(0))^2 \rangle = 2k_B T(m\gamma)^{-1}t$ for a standard Brownian diffusion. In case of ABM, due to the inverse-proportional dependence on the noise intensity D (cf. Eq. (1)), weak noise gives rise to large mean square displacement which is one of the peculiar properties of the motion [3].

From now on we will consider only one-dimensional problems. First we analyze the deterministic equations for several instructive special cases (for simplicity of derivations we assume $m = 1$):

$$\ddot{x}(t) + U'(x) + [\gamma - de(t)]\dot{x}(t) = F_0 \quad (14)$$

$$\dot{e}(t) - q + ce(t) + de(t)\dot{x}^2(t) = 0 \quad (15)$$

Here F_0 stands for a possible tilt of the potential. As a zeroth-order approximation we first neglect in Eq.(14) the term $U'(x) = 0$ and we adiabatically eliminate the energy term from the second equation by approximating $\dot{e} = 0$:

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= -[\gamma - de(t)]v + F_0 \\ \dot{e}(t) &= 0 \rightarrow e = \frac{q}{c + dv^2} \end{aligned} \quad (16)$$

When treating the set of the above equations by use of the equilibrium condition (vanishing of the dissipation term in the second equation) which requires $e_0 = \gamma/d$ we assume that the stability flux of energy counterbalances the friction term:

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= F_0 \\ e &= e_0 = \frac{\gamma}{d} = \frac{q}{c + dv_0^2} \end{aligned} \quad (17)$$

The above set of equation implies now that $F_0 = 0$.

We will take later this exact solution (with $F_0 = 0$ and $U'(x) = 0$) as the starting point of a perturbation theory. The bifurcation parameter of our problem is β . For $\beta \geq 0$, the system is driven to non-equilibrium states (note that this case requires pumping of energy from the reservoir) and has all together three stationary states of the velocity: $v = 0$, $v = v_0$ and $v = -v_0$.

We consider now the case of a constant tilt by means of the additive force

$$F_0 = -a. \quad (18)$$

Here a is the slope of an equivalent potential $U_0(x) = ax$. We will mostly focus on a positive slope $a > 0$, $F_0 < 0$. Let us first consider the case in the absence of an additional ratchet potential i.e. $U(x) = 0$. This problem still admits an exact solution. Without an energy flux q from the reservoir, the particle would fall down (if $a > 0$ from right to left). Including the reservoir provides the possibility of uphill motions. The condition of stationary motion under the action of this force leads to the cubic equation

$$\gamma dv_0^3 - F_0 dv_0^2 + (c\gamma - qd)v_0 - F_0 c = 0 \quad (19)$$

The solutions may be found graphically (see Fig. 1). If we assume that dissipation c and the slope a are so small that $ac = -F_0 c$ may be neglected, the solution reads

$$v_0 = \frac{F_0}{2\gamma} \pm \sqrt{\frac{F_0^2}{4\gamma^2} + \frac{q}{\gamma} - \frac{c}{d}} \quad (20)$$

Altogether, in the general case we have a cubic equation

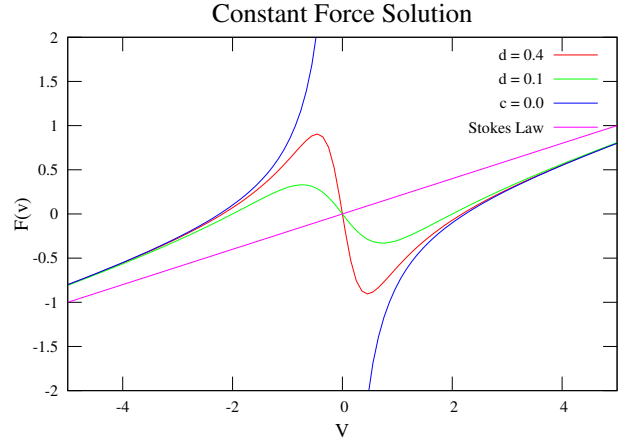


Fig. 1. Stationary solution: The force $F(v) = F_0 = -a$ as a function of the velocity for $\gamma = 0.2$ and 2 fixed d -values ($d = 0.4$ and $d = 0.1$ with $c = 0.1$) and the asymptotic curve with $c = 0$. The comparison is made with the Stokes law $F(v) = \gamma v$. The solution to Eq. (19) representing free motion corresponds to the roots on the axis $F(v) = 0$

for the stationary velocities, which is easy to solve numerically, and in some special cases, also analytically. Following the structure of the linear potential U_0 , the downhill motion exists in all cases and for our standard choice $a > 0$; $F_0 < 0$ the downhill motion is directed to the left. Remarkably, in the case of positive energy input $q > 0$ also a stationary uphill motion may exist $v_0 > 0$, provided the force driving downhill is not too large. For example, if $a = 1$; $F_0 = -1$, the trivial downhill solution is $v_0 = -5$ and the stable uphill solution is $v_0 = +0.5$ for $d = 1$; for $d = 0.3$ no uphill solution exists. It is interesting to mention that the uphill motion may exist even without any ratchet effects provided the driving is sufficiently strong. Still the question remains, what is the influence of the ratchet potential on the directionality of transport and what is the mechanical efficiency of the system.

This brief examination allows us to conclude about the minimum set-up conditions for construction of a ratchet-type potential in which the unidirectional current can be obtained:

- (i) the average value of the flatter slope of the potential should be in the range where the uphill motion is possible, and
- (ii) the average value of the steeper slope should not allow the uphill motion.

Under these conditions the particle can go uphill from left

to right and, since the motion backwards is not possible, we get a unidirectional movement. We will use this construction as a rule of thumb in order to find the conditions for directed transport in one dimensional periodic structures.

2.3 Effect of white noise in the mechanical equations with constant force

Having in mind biological applications where typically some transfer from chemical to mechanic or electric energy appears in the presence of random fluctuations, we will study now ratchets which are connected to an energy reservoir under the influence of noise. As a generalization of Eq.(14)

$$\frac{dv(t)}{dt} + \gamma v(t) + U'(x) = F_0 + de(t)v(t) + \sqrt{2D}\xi(t) \quad (21)$$

The equation for the energy depot remains instead exactly Eq.(15). For special case when $U'(x) = 0$, $F_0 = 0$ and $\dot{e} = 0$, the corresponding Fokker-Planck equation may be solved and the solution is given by Eq. (11). When including a constant tilt $F_0 = -a < 0$, the stationary Fokker-Planck equation may also be solved exactly. The solution gives now an asymmetrical distribution with two maxima corresponding to the deterministic stable flux velocities (see Fig. 2):

$$P_0(v) = C \exp \left[-\frac{\gamma v^2}{2D} - av + \frac{q}{2D} \log(1 + \frac{d}{c} v^2) \right]. \quad (22)$$

The shape of the stationary probability density demon-

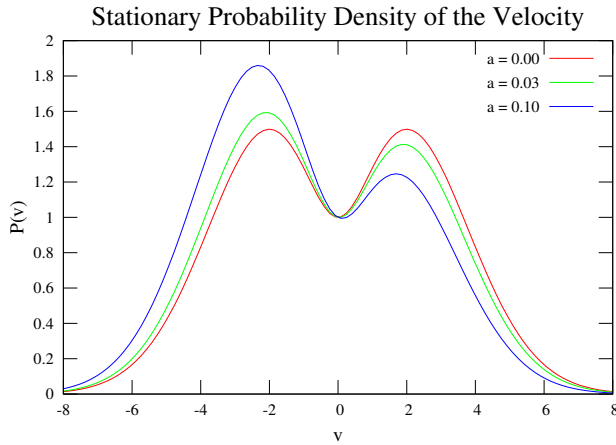


Fig. 2. Example of the asymmetric probability distribution of the asymptotic velocity under a ratchet in the presence of a tilt for different values of the constant force intensity a . The tilt of the potential gives rise to the asymmetry of the distribution.

strated in Fig.2 shows that under the action of a constant force directed to the left ($a > 0$), flows in both directions

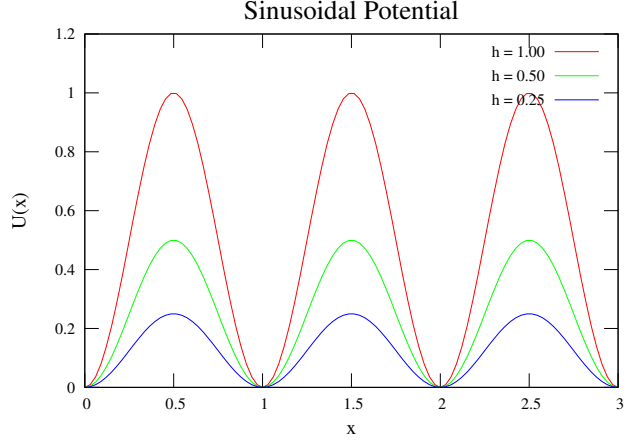


Fig. 3. Sinusoidal potential with parameter $h = 1.0, 0.5, 0.25$.

are possible, however with a different probability: Flows directed to the right are less probable than those oriented to the left.

3 Ratchets coupled to energy sources

3.1 Models of inertia ratchets

In a series of recent papers [22,23] various aspects of the ABM energetics in an external potential have been analyzed. In order to investigate further the motion of an ensemble of pumped Brownian particles in periodic fields, we consider two simple models of smooth 1-dim potentials: the symmetric sinusoidal potential (see Fig.3):

$$U(x) = \frac{h}{2}[1 - \cos(2\pi x)] \quad (23)$$

and the asymmetric ratchet potential (See Fig.3 and Fig.12) introduced by Mateos and Machura [24,25]:

$$U(x) = h\{0.499 - 0.453\{\sin[2\pi(x + 0.1903)] + 0.25 \sin[4\pi(x + 0.1903)]\}\}. \quad (24)$$

We first address the problem of the classical deterministic dynamics of a particle in those potentials. We construct the bifurcation diagram and identify the origin of the current. By analyzing stochastic influences, we detect noise-induced directionality of the current.

3.2 Sinusoidal Ratchets in the trapped regime

We study first oscillations around $x = 0$. In this case the potential can be approximated by a parabolic one

$$U(x) \simeq h\pi^2 x^2 = \frac{1}{2}\omega_0^2 x^2. \quad (25)$$

and for a positive value of the bifurcation parameter $\beta > 0$ the system displays self-oscillating solutions. By assuming their form as

$$v(t) = a \sin(\omega t - \alpha), \quad (26)$$

and substituting into the set of evolution equations, we may determine the amplitude a . For small β a standard derivation of a periodic solution yields $a = (2\beta)^{1/2}$ and $\omega = \omega_0$.

In Fig. 4 the plot of the amplitude of the asymptotic velocity a as a function of the parameter q is displayed. We see that small amplitudes follow predicted root law whereas divergence between analytical and numerical results at higher values of q are due to a breakdown of the parabolic approximation of the potential. For higher val-

ues it differs significantly from the value predicted in this approximation ($d_{E,a}$) (See Fig.8).

For particles entrapped in the potential well and performing sustained oscillations one can derive an analytical expression for the value of energy in the energy-reservoir. The starting point for the derivation is an assumption that at a moderate energy transfer parameterized by d , a confined closed orbit occurs in a potential well. Let's assume that this trajectory is characterized by a sinusoidal velocity:

$$\dot{x}_\infty(t) = a \sin(\omega t), \quad (29)$$

After substituting $\dot{x}_\infty(t)$ in Eq.(15) and integration, the analytical expression for the depot energy $e(t)$ takes on the form:

$$e_\infty(t) = (qW(t) + e_0)e^{-\eta(t)} \quad (30)$$

where

$$W(t) = \int_0^t e^{\eta(t')} dt' \quad (31)$$

and

$$\eta(t) = (c + da^2/2)t - \frac{da^2}{4\omega} \sin(2\omega t). \quad (32)$$

The integral Eq.(31) can be evaluated in the long time limit and the result implemented again to the formula Eq.(30) leading to an asymptotic expression for the depot energy

$$e_\infty(t) = \frac{q}{c + da^2/2} \exp\left(\frac{da^2}{4\omega} \sin(2\omega t)\right). \quad (33)$$

which averaged over the time becomes:

$$e_\infty = \langle e_\infty(t) \rangle_\tau = \frac{q}{c + da^2/2} \left\langle \exp\left(\frac{da^2}{4\omega} \sin(2\omega t)\right) \right\rangle_\tau. \quad (34)$$

Here brackets represent the time average

$$\langle f(t) \rangle_\tau \equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau f(t) dt \quad (35)$$

In a first approximation¹ we can use

$$\left\langle \exp\left(\frac{da^2}{4\omega} \sin(2\omega t)\right) \right\rangle_\tau \approx 1. \quad (36)$$

due to the average $\langle \sin(2\omega t) \rangle_\tau = 0$. This means that

$$e_\infty \approx \frac{q}{c + da^2/2}. \quad (37)$$

¹ This approximation holds only for $\frac{da^2}{4\omega} \ll 1$, which is a valid value for our case. A more general value can be found as follow: we have that $\langle e^{\frac{da^2}{4\omega} \sin(2\omega t)} \rangle_\tau \in [e^{-\frac{da^2}{4\omega}}, e^{\frac{da^2}{4\omega}}]$, so we can put as approximation the mean value between the two extremes of the exponential function: $\Rightarrow \langle e^{\frac{da^2}{4\omega} \sin(2\omega t)} \rangle_\tau \approx \cosh(\frac{da^2}{4\omega})$. In this more general case, the relation between the parameters is: $\frac{q}{c + da^2/2} \cosh(\frac{da^2}{4\omega}) \approx \frac{\gamma}{d}$. This relation is not simple to invert and also requires ω as an input value to obtain a .

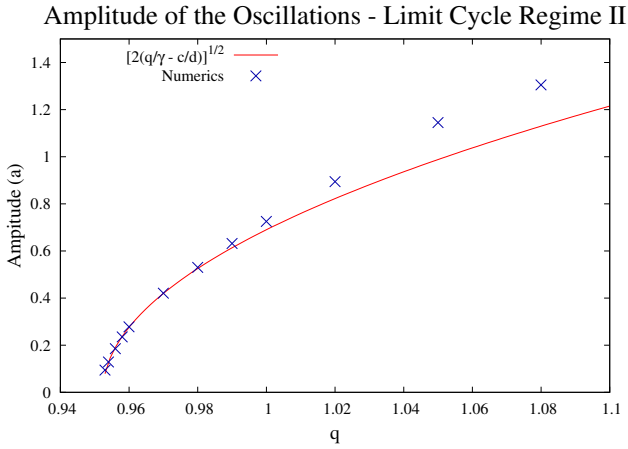


Fig. 4. Amplitude of the limit cycle as a function of driving parameter q for different values beyond the critical values (symbols) in comparison with the theoretical result (full line). We used a ratchet with $h = 1$, driving parameters $\gamma = 0.2$, $c = 0.1$, $d = 0.021$. For amplitudes larger than around half of the maximal amplitude, the theory breaks down due to significant deviations of the sine-potential from a parabola.

ues we observe a bifurcation from a limit cycle to an open trajectory. The transition to open trajectories is expected in the region where the kinetic energy exceeds the maximal potential energy:

$$\frac{1}{2}v_0^2 = \frac{1}{2} \left(\frac{q}{\gamma} - \frac{c}{d} \right) \geq h \quad (27)$$

Consequently, in what follows, we use the energy transfer parameter d as an order parameter in our study. The equality sign ($=$) in the above expression defines the value of the energy exchange parameter d giving rise to a bifurcation between stable oscillations and the flux regime. We denote this value d_E .

$$d_E = \frac{d_c}{1 - d_c h/c} \quad (28)$$

where $d_c = \gamma c/q$. The above expression, as based on the parabolic approximation of the potential, gives only a rough estimation of d_E and is no longer valid in the dynamical region where the transition from stable oscillations (trapped trajectories) to the flux regime takes place. As a consequence, the numerically evaluated parameter ($d_{E,n}$)

which differs from Eq.(17) by a factor $1/2$. On the other hand, by assuming close-to-equilibrium condition (dissipation term vanishing over the time average) in Eq. (14) we can evaluate:

$$\langle \gamma - de_\infty(t) \rangle_\tau = 0 \quad (38)$$

This means that:

$$e_\infty = \frac{\gamma}{d}. \quad (39)$$

Comparing Eq.(14) and Eq.(39), we have a relation between the parameters of the equations and the amplitude a of the limit velocity of the particle:

$$\frac{q}{c + da^2/2} = \frac{\gamma}{d} \Rightarrow a = \sqrt{\frac{2q}{\gamma} - \frac{2c}{d}} = \sqrt{2\beta}. \quad (40)$$

This predicted value for a is very close to that found by the numerical solution of the equations. From the former equation is it possible to evaluate the limit threshold giving the stable oscillation of the system. In fact, by putting $a = 0$ we obtain the value

$$d_c = \frac{\gamma c}{q}. \quad (41)$$

To resume the present result, we have, for $d_c < d < d_E$:

- stable oscillation of $v(t)$ with amplitude a
- stable oscillation of $x(t)$ in a certain well of the potential with amplitude $a/2\pi\omega$
- oscillating stationary behavior for $e_\infty(t)$ with frequency $\omega_e = 2\omega$,

while for $d \leq d_c$ we have:

- limit value $x(t)$ in a certain final position x_f
- decreasing of $v(t)$ ($a = 0$)
- damped oscillating behavior with saturation for $e_\infty(t)$ (see Eq.(33) for $a^2 = 0$)

Results of numerical evaluation, together with the analytical result Eq.(33), are plot in two figures below (Figs.5, 6). As it can be deduced from the simulations, motion in the periodic ratchet potential leads to oscillatory behavior of the energy $e(t)$. That refrains us from using strictly the elimination scheme based on the assumption $\dot{e}(t) = 0$. Instead, the periodic variation of $e(t)$ leads to an average (over time) constant value of e_∞ that differs from the value predicted in Eq.(17).

3.3 Sinusoidal ratchets in the flux regime

We will try first a perturbation theory developing the expression of the velocity of our system:

$$\begin{aligned} v &= v_0 + v_1(t) + \dots; \\ e &= e_0 + e_1(t) + \dots \end{aligned} \quad (42)$$

For large driving and small forces ($U'(x) \approx 0$) the particles move as free and there are two attractors of the velocity

$$\begin{aligned} v_0^+ &= \sqrt{\beta}, \\ v_0^- &= -\sqrt{\beta} \\ e_0 &= \frac{\gamma}{d} \end{aligned} \quad (43)$$

$x_0 = 0.0, v_0 = 6.0, e_0 = 2.0 \mid d = 0.024, \gamma = 0.20, c = 0.1$

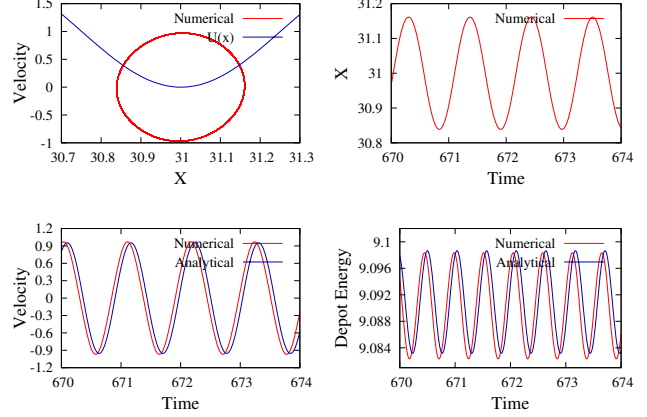


Fig. 5. Asymptotic behavior of the system in the trapped case with limit cycle ($d_c < d < d_E$). $a = \sqrt{\frac{2q}{\gamma} - \frac{2c}{d}}$. Graphs of time-dependent energy represent variation of the depot energy $e(t)$.

$x_0 = 0.0, v_0 = 6.0, e_0 = 2.0 \mid d = 0.012, \gamma = 0.20, c = 0.1$

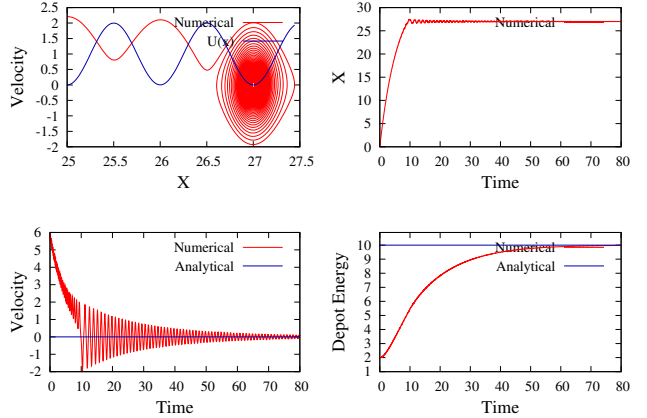


Fig. 6. Asymptotic behavior of the system in the trapped case with zero limit ($d \leq d_c$) and imaginary parameter a . Graphs of time-dependent energy represent variation of the depot energy $e(t)$.

We take these solutions as the first term in a perturbation series. Inserting this *zero*- approximation into the Eq. 14, we have:

$$\dot{v}_1(t) = \frac{dv_1(x)}{dx} \frac{dx}{dt} \approx \frac{dv_1(x)}{dx} v_0 = -U'(x) \quad (44)$$

From which, integrating in x , we have the solution:

$$v_1(x)v_0 \approx -U(x) + Const \quad (45)$$

and therefore, up to the first order:

$$v_{(1)}(x) = v_0 + v_1(x) \approx v_0 - \frac{U(x)}{v_0} + \frac{Const}{v_0}. \quad (46)$$

The choice of the constant, is made in order to have a the mean value of the potential equal to 0 (See Eq. (24)). The

value of the constant is then $Const = 0.499h$. With this choice we obtain, up to the 1st order of approximation:

$$v_{(1)}(x) \approx v_0 - \frac{U(x)}{v_0} + \frac{0.499h}{v_0}. \quad (47)$$

The above expression is valid, in principle, for any shape of differentiable potential ratchets.

Taking into account the Eq. 47, we can make the assumption for our asymptotic velocity:

$$\dot{x}_\infty(t) = b + a \sin(\omega t), \quad (48)$$

the analytical expression for the $e(t)$ is then:

$$e_\infty(t) = (qZ(t) + e_0 e^{-2dba/\omega}) e^{-\xi'(t)} \quad (49)$$

where

$$Z(t) = \int_0^t e^{\xi(t')} dt' \quad (50)$$

and

$$\xi(t) = (c + db^2 + da^2/2)t - \frac{\zeta(t)}{\omega}. \quad (51)$$

with

$$\zeta(t) = 2db a \cos(\omega t) + \frac{da^2}{4} \sin(2\omega t). \quad (52)$$

Because the term $(c + db^2 + da^2/2)$ is greater than zero, the equation has a non vanishing and non diverging asymptotic behavior. The asymptotic expression we can extract from the equation is now:

$$e_\infty(t) = \frac{q}{c + db^2 + da^2/2} e^{\zeta(t)/\omega}. \quad (53)$$

The expression for $e_\infty(t)$ presents in the exponential two oscillating functions with two different frequencies (ω and 2ω). Because the coefficient of the cosine function is greater than that of the sine, the observable frequency in the reservoir energy is the same than the velocity one, while in the trapped case we have only the frequency 2ω for the asymptotic energy. Fig.7 shows the behavior of this expression compared with that one obtained by numerical evaluation. The agreement is very good. The parameter a and b can be evaluated by means of the comparison with the Eqs.(48) and (47), while ω has been extracted from the numerical evaluation of the limit velocity $v_\infty(t)$.

3.4 Influence of external forces and noise

Assuming that the external force is different from zero, we put a certain bias to the right or left direction. A particle which is able to go uphill at the cost of the supply from the reservoir energy may convert this energy into mechanical or electrical energy and perform work. This simple motor device is of particular interest in nanobiotechnology, where the reservoir energy is in most realistic cases just the chemical energy of reaction.

Among various ratcheting devices, a special class are so called staircase ratchets. This type of ratchets may find

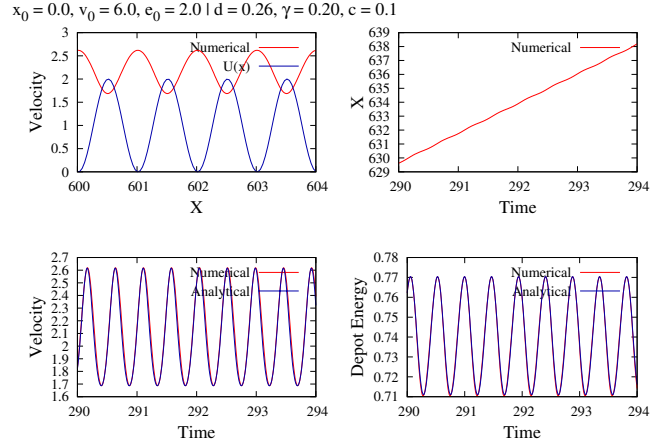


Fig. 7. Case of asymptotical flux. Numerical and analytical behaviors are quite superimposed. Differently from the trapped case, the energy oscillates mainly with the same frequency of the velocity.

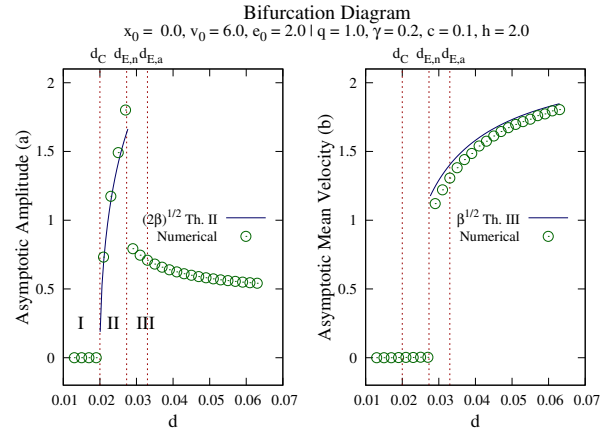


Fig. 8. Bifurcation diagram for the amplitude (left hand side) and the mean value (right) of the asymptotic velocity. The comparison between the predicted values and the measured ones are plotted. The three region I, II, III, represents the different dynamical regimes as a function of the order parameter d . The indicated threshold values $d_{E,n}$, $d_{E,a}$ represents respectively the numerical and analytical evaluation (assuming the harmonic potential profile) of the escape bifurcation parameter d_E (see Eq.28)

applications to understand and design biological steppermotors [15,17]. Usually steppermotors have two phases: (i) a power stroke where the legs move against a force and (ii) a phase of free motion or diffusion. We propose to model those by a staircase ratchet having a steep and a flat region.

As a simple example we study the potential obtained by a sinusoidal ratchet with a very strong tilt (See the first plot in Figs. 9 and 10):

$$U(x) = h \left[x - \frac{1}{2\pi} \sin(2\pi x) \right]. \quad (54)$$

Here the parameter h denotes the height of one step. As can be inferred from Figs. 9 and 10, the readjustment of the exchange energy parameter d can drive the system uphill in the staircase ratchet. Fig. 10 presents a longer stabilization time because we are close to the critical d_{cr} value below which the uphill motion is not observed. In fact, for $d = 1.3$ we observe only a sliding down motion of the system. Moreover, in the chosen potential the initial velocity plays a key role. Initial velocities lower than the limit mean value (equal to 1 in Figs 9 and 10), give rise to stopping down motion only.

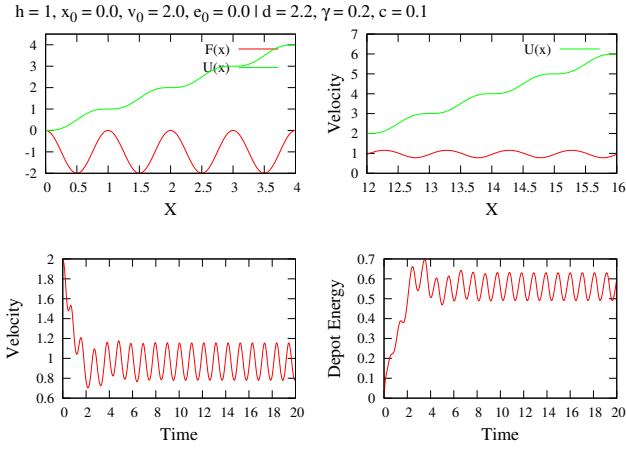


Fig. 9. Active motion on staircase ratchets for a rather large value of the strength of driving $d = 2.2$.

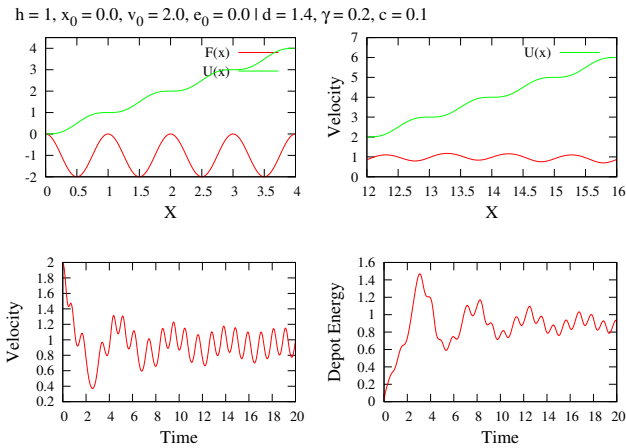


Fig. 10. Active motion on staircase ratchets for a smaller value of the driving which is near to the threshold of uphill motion $d = 1.4$.

As a last result for the sinusoidal-like ratchet, we present numerically evaluated statistics of the right trajectories as a function of the noise intensity for both: the tilted and tilt-free ratchet. In Fig. 11 we plot the case of sinusoidal potential with and without additional constant force in

the equation motion. As expected, different white noise intensities don't lead to any asymmetry in the statistics of the flux directionality (right or left) in the absence of the constant force ($F_0 = 0$). In contrast, the additional constant force, strongly affects the motion. For very low values of noise, such as in the deterministic regime, we observe that superposition of both forces added gives rise to different flux directionality for the set of parameters used.

When increasing the noise intensity in the region $D \approx [10^{-9}, 10^{-6}]$, a non-monotonic behavior of the fraction of right-oriented trajectories N_{Right}/N_{Tot} as a function of the noise intensity is observed. By further increasing the noise $D \approx [10^{-6}, 10^{-3}]$, a region of strong preference towards left-oriented trajectories is detectable, giving the expected behavior of the flux in agreement with the applied constant force. Still higher values of noise intensity blurred the picture and the rectifying properties of the system are no longer detectable ($N_{Right}/N_{Tot} \approx 0.5$).

This *stochastically driven directionality* of the sinusoidal ratchet system in the presence of an additional tilt appears to be a generic effect and will be further discussed (for asymmetric ratchets) in the forthcoming section, where similar statistics of N_{Right}/N_{Tot} events has been evaluated.

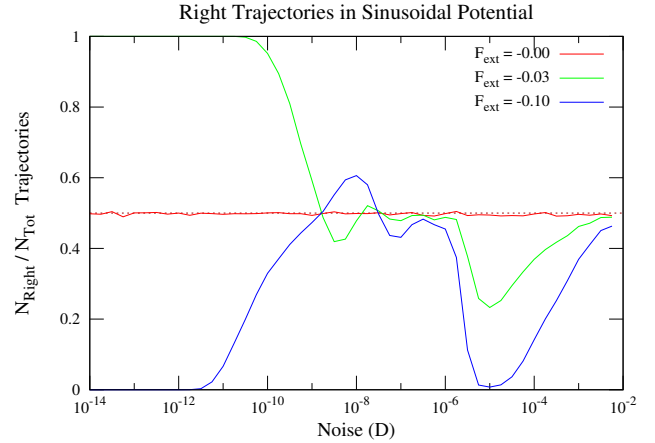


Fig. 11. Statistics of the right/left trajectories for the sinusoidal ratchet with and without the presence of different constant forces as a function of noise-intensity.

4 Asymmetric Smooth Ratchet Potential

4.1 Analytical results from perturbation theories

As in the case of the sinusoidal potential, also for the asymmetric ratchet case we observe three different regimes depending on the depot-energy influx to the mechanical motion:

- (i) the state of complete rest (point attractor of the dynamics),
- (ii) sustained oscillations in one well (bounded attractor),

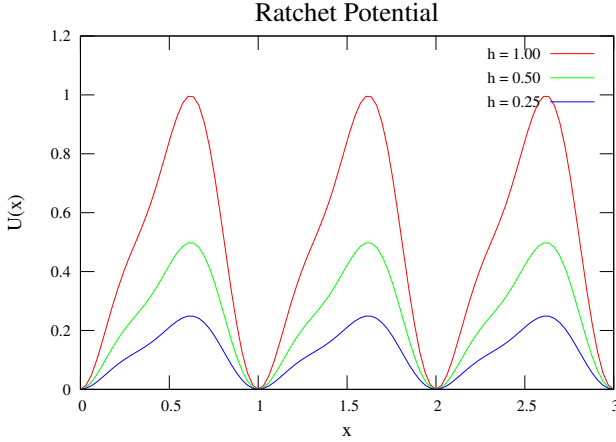


Fig. 12. Ratchet potential obtained adding two sinusoidal functions for different height $h = 1.0, 0.5, 0.25$ (Eq. 24).

(iii) flux regime (open attractors).

The bifurcation plot of these regimes is isomorphic to that one of the sinusoidal potential and it is shown in Fig.8. We study here only the flux regime which is the most interesting regime for rectifying ratchet systems. The analytical expressions for the trapped cases (corresponding to the harmonic approximation of the potential), are identical to those reported in the previous chapter.

Examples of trajectories in the flux regime are given in Fig.13,14. By inspection of these plots we conclude that the change in the right and left asymptotical velocity is not monotonically dependent on the energy transfer parameter d .

The analytical evaluation of the velocity and the energy in the ratchet case, follows the same scheme used for the sinusoidal potential. Using the expression of the velocity derived in the perturbation treatment (Eq. (47)), with the ratchet of the Eq.(24), we can proceed with the evaluation of the analytical asymptotic behavior of the depot energy using the expression of the velocity written in the following way:

$$\dot{x}_\infty(t) = b + a \sin(\omega t) + f \sin(2\omega t), \quad (55)$$

the formal analytical expression for the $e(t)$ is then:

$$e_\infty(t) = [qY(t) + e_0 e^{-db(f+2a)/\omega}] e^{-\zeta(t)} \quad (56)$$

where

$$Y(t) = \int_0^t e^{\zeta(t')} dt' \quad (57)$$

and

$$\zeta(t) = (c + db^2 + \frac{da^2}{2} + \frac{df^2}{2})t - \frac{\theta(t)}{\omega}, \quad (58)$$

with

$$\begin{aligned} \theta(t) = & 2dba \cos(\omega t) - daf \sin(\omega t) + \\ & + dfb \cos(2\omega t) + \frac{1}{4}da^2 \sin(2\omega t) + \\ & + \frac{1}{3}dfa \sin(3\omega t) + \frac{1}{8}df^2 \sin(4\omega t). \end{aligned} \quad (59)$$

Because the term $(c + db^2 + da^2/2 + df^2/2)$ is again greater than zero, the equation has a non vanishing and non diverging asymptotic behavior. The asymptotic expression we can derive from the equation is then:

$$e_\infty(t) = \frac{q}{c + db^2 + da^2/2 + df^2/2} e^{\theta(t)/\omega}. \quad (60)$$

The expression for $e_\infty(t)$ contains in the exponential six oscillating terms with four different frequencies ($\omega, 2\omega, 3\omega$, and 4ω). The relative weight of the higher frequencies are low because of the coefficient of these terms and also because the value of the coefficient f which is equal, in our potential, to one forth the coefficient b . The relevant oscillating term is then that one with frequency ω , the others representing less significant harmonics.

Performing the average of the asymptotic energy $\langle e_\infty(t) \rangle_\tau$ as made with the sinusoidal potential, and equalizing it to the value γ/d , we can simplify the expression for the energy $e_\infty(t)$ as:

$$e_\infty(t) = \frac{\gamma}{d} e^{\theta(t)/\omega}. \quad (61)$$

that is the expression used in our predictions. Fig.13 shows

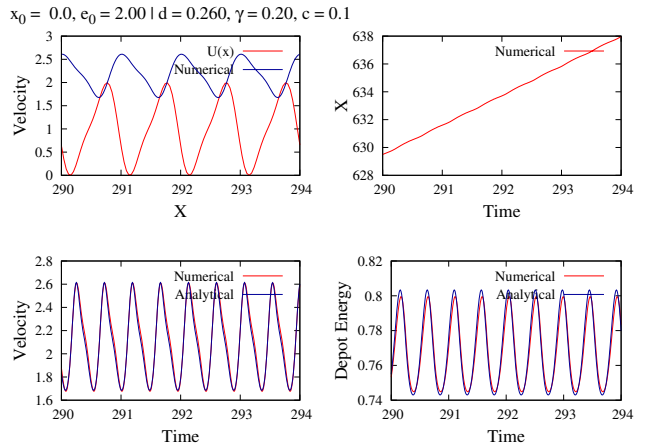


Fig. 13. Asymptotic behavior of the system in the flux case with the usage of the Mateos asymmetric ratchet potential plotted in Fig.12.

the behavior of this expression compared with that one obtained by numerical evaluation. Even in this asymmetric case, the agreement is extremely good. The parameters a, b, f come from the expression of the velocity, and ω has been extracted from the numerical evaluation of the limiting velocity $v_\infty(t)$. Otherwise, ω can be also predicted by means of the mean flux velocity $\langle v_\infty(t) \rangle_\tau = b$ using the relation:

$$bT = \frac{b}{\nu} = \frac{2\pi b}{\omega} = L = 1 \Rightarrow \omega = 2\pi b, \quad (62)$$

where T is the period of the oscillations, ν the corresponding frequency and L is the length of the ratchet periodicity.

4.2 Results of simulations

Numerical simulations performed by Tilch et al. (1999) have documented that, at least for ratchet models with piecewise linear potentials, the onset of a directed net current appears in two different directions. Similar behavior is registered in this study: at sufficiently large values of driving, close to the stationary states v_0^+ and v_0^- , the dynamical system possesses open attractors corresponding to the left or right current states. As we can see in

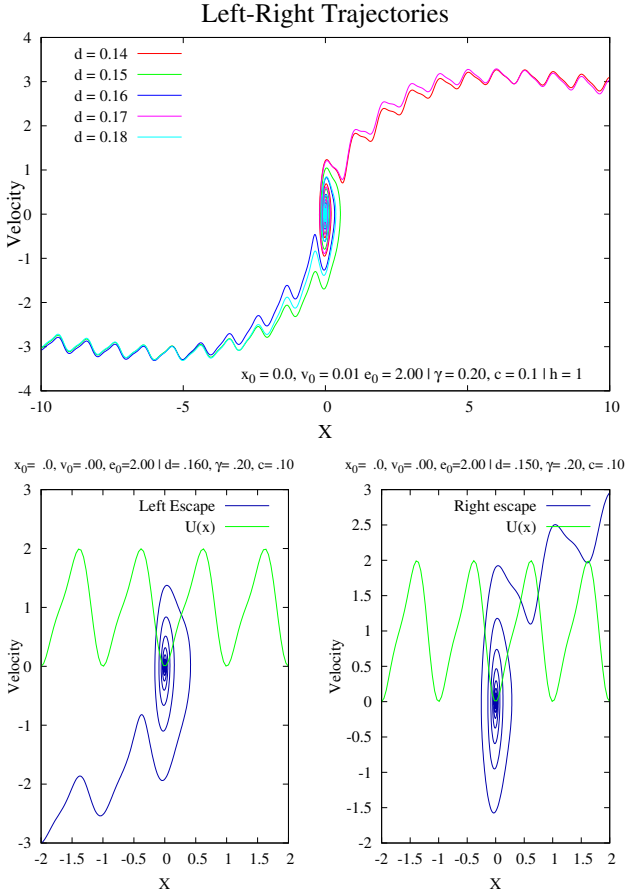


Fig. 14. Examples of escape events from the well of the ratchet-potential. Relatively small variations of the energy transfer parameter d can induce different directionality of flux.

Fig. 14, the ratchet driven by active friction with a strong depot-particle coupling ($d > d_E$) possesses 2 momentum-dependent attractors. Slight variations of the intensity d result in changes of the flux directionality, especially in the domain of low noise-strengths (cf. Fig. 15) where the dynamics follows the trend observable in a deterministic system. The overall pattern, however, does not reveal any systematic tendency. In case of stochastic dynamics, two asymptotical velocities can be compared with two modal values (most probable ones) of the stationary probability density $P_0(v)$. Here, instead of examining positions of maxima of $P_0(v)$, we have analyzed portion of trajectories

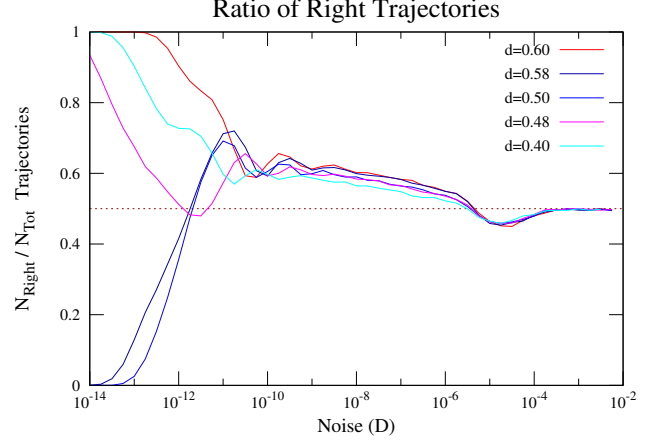


Fig. 15. Fraction of right-directed trajectories N_{Right}/N_{Tot} out of the total number of analyzed cases $N_{Tot} = 5 \times 10^4$. Directionality of the asymptotic velocity is displayed as a function of the noise intensity.

whose long time evolution results in a preferred direction of motion (Fig. (15)). Closer inspection of Fig. (15) allows to detect noise-induced changes in the directionality of current. For very low noise intensity, a deterministic scenario prevails and the direction of current is decided by the deterministic dynamics (cf. Fig.(14)). In contrast, at increasing values of the noise intensity ($D \simeq [10^{-12}, 5 \cdot 10^{-4}]$) the system exhibits a tendency to move towards right. At still higher values of $D \simeq [5 \cdot 10^{-4}, 10^{-2}]$, the preferred asymptotic direction changes to the left. Eventually, for values of $D \simeq 10^{-3}$ the motion of the system becomes fully delocalized resulting in equal ratios of trajectories going to the left and right.

4.3 Tilted ratchets

First we discuss the existence of an unidirectional ratchet. Studying a Mateos ratchet it is allowed a choice of parameters such that the average of the smaller slope (increasing left to right) can still be overcome by the driving mechanism. However the large slope (from right to left) is too large to be overcome. In other words, there exists an uphill solution for the smaller slope and no uphill solution for the larger slope. This prevents any possibility to go left in our case. The ratchet-system is acting then as a unipolar, rectifying device.

Under tilted ratchets we understand ratchets with a constant average slope. In other words we have a global incline of the ratchet which is due to some constant average force. This may model a constant external load against which the ratchet has to do work. We mention that several authors considered also the case of oscillating tilts. We are interested in doing work against a load, therefore consider here only constant external slopes.

In Fig. 16 we give an example of an uphill motion against a force (here $F = 0.03$). The load force is in the

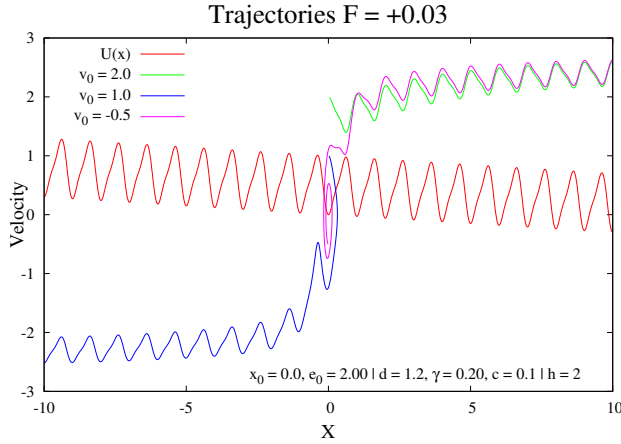


Fig. 16. Examples of uphill flux on tilted ratchets. The load force is directed left to right.

example directed left to right. We see that in dependence on the initial conditions both directions may be realized.

5 Applications

The investigated systems may be of interest for the modelling of molecular motors which are able to convert chemical energy into mechanical energy (work). We see possible applications to proton pumps, the rotating motors connecting with the work of ATP-ase [13,14] and also to step motors as proposed by Bier [15,17].

Molecular motors are nanotechnological objects being the result of biological evolution. All molecular motors use the energy quantum connected with the synthesis or hydrolysis of the nucleotides ATP/ADP or the difference of the electrochemical potentials on the cytoplasm membrane. Standard models of molecular motors are based on the Smoluchowski equations for discrete systems having several states which correspond to attachment or detachment [13,14]. Many models have been developed which follow similar lines. We follow in this work another route which is based on Hamiltonian ratchets. We studied Hamiltonian ratchets which are connected to an energy reservoir and gave special attention to possible applications to molecular motors. We investigated in detail the motion of a particle against a gradient of the potential i.e. uphill motion under conditions where the external force is pointing downhill. The general schema is the following: chemical energy is absorbed in the form of ATP and introduced into our "motor" increasing the reservoir of $e(t)$ by a certain amount. This is modelled here by a continuous inflow q . In some other work we develop a more refined model based on the assumption of discrete energy quanta, representing the absorption of one molecule ATP [18]. The absorbed energy flows to the "motor" and is transformed into mechanical or electrical potential energy. This could e.g. model the increase of the energy of protons by transport through the membrane.

In the case of the ATP-ase motor, in one of the direction of its rotational kinematics, the enzyme ATP-ase hydrolyzes ATP into ADP and anorganic phosphate-Pi, releasing energy and moving protons. The work of F_0F_1 -ATP-ase is connected with the rotation of a "rotor". The idea about a "rotor" corresponds to our knowledge about the structure (see Fig. 17). In our model of active Brown-

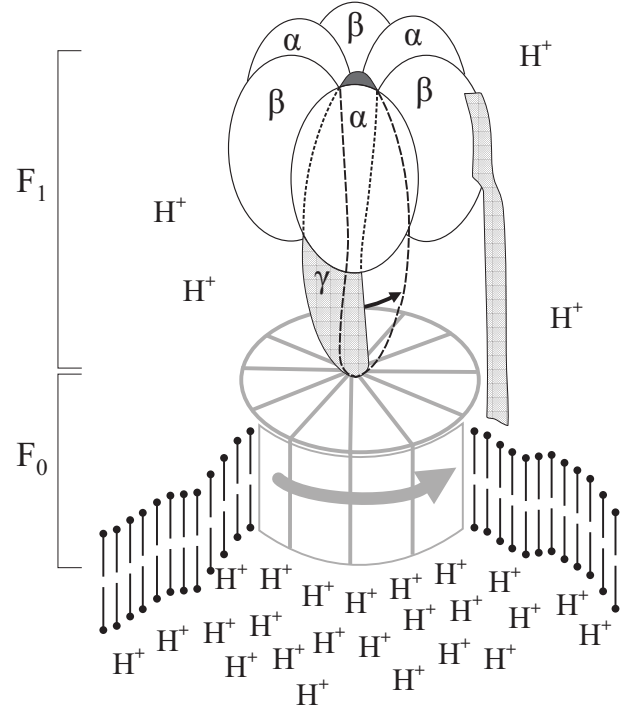


Fig. 17. Scheme of the molecular motor F_1F_0 -ATPase-synthase. The complex F_0 which is imbedded into the membrane is responsible for the transport of protons through the membrane. The complex F_1 sitting on the membrane is responsible for the catalytic functions during the synthesis / hydrolysis of ATP. The figure has been adapted from an online publication of the Royal Swedish Academy of Sciences (http://nobelprize.org/nobel_prizes/chemistry/laureates/1997/press.html).

ian particles the variable x has to be interpreted then as the rotation angle of the rotor.

Another possible application may be to model step motors, as studied e.g. by Bier [15,16,17]. Here the motion of molecular legs is composed by two phases. The first phase is the power stroke where the system works against a force, and the second phase is the free or diffusive motion. One possibility to model such two-phase motions is to use staircase-like ratchets defined by Eq.(52). Another possibility is to develop ratchet models based on two active particles coupled by a spring. Step motor models of this type, based on overdamped ratchet motion, were first studied by Derenyi and Vicsek [26].

6 Summary

In this work we analyzed a mechanical system with inertia subjected to a dissipative forcing having two terms: one passive damping and an 'active' contribution providing energy to the system by means of an energy supply described in an additional coupled equation. The system has been studied under the influence of smooth ratchet potentials: symmetrical (sinusoidal potential) and asymmetrical (Mateos-type potential and tilted ones). The analytical and numerical evaluation of the equations has been found for both the asymptotical velocity of the mechanical system and the depot energy. The system presents bifurcations of the asymptotic velocity as a function of the energy transfer parameter d . The three regimes found correspond to: 1) relaxation in a potential minimum (vanishing motion); 2) oscillating motion in a well (limit cycle), and 3) flux motion with two values of the asymptotic velocity. The motion in the flux regime is then possible in two directions, even in the presence of a tilt in the potential. The numerical simulations of the system under the action of white Gaussian fluctuations show the effect of noise-controlled directionality of the motion.

Possible applications of the ABM system in modelling molecular motors connected to the *ATP* synthesis/hydrolysis have been briefly discussed.

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